1,2-Diphenylhydrazine 122-66-7 | DTXSID7020710

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 31.8 days

Global applicability domain: Inside

Local applicability domain index: 4.50e-01

Confidence level: 8.15e-01

Nearest Neighbors from the Training Set

Image not found

Anthracene

Measured: 64900 Predicted: 105 Image not found

Fluorene

Measured: 6090 Predicted: 42.2 Image not found

1,4-Dimethylnaphthalene

Measured: 511 Predicted: 13.7

Image not found

Phenanthrene Measured: 5460 Predicted: 75.9 Image not found

1-Methylnaphthalene Measured: 164

Predicted: 12.0